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Basics of Data Processing

Scott Calvin
Sarah Lawrence College

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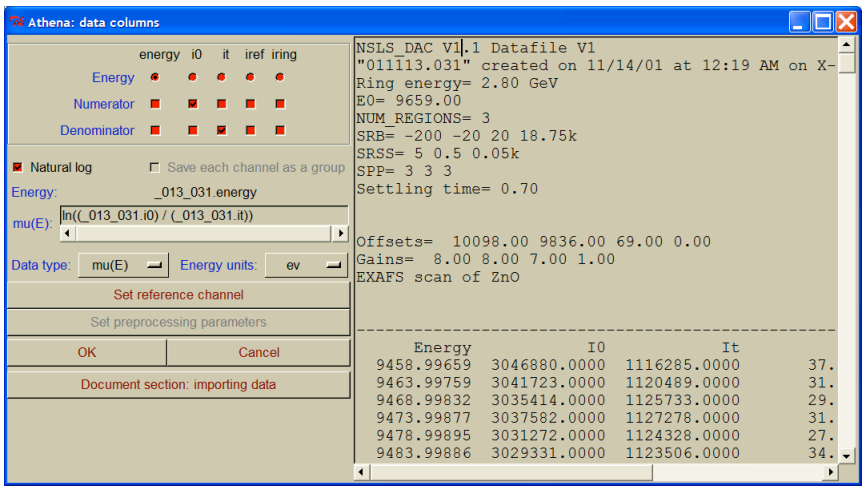
Importing Raw Data in Athena



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What This Talk Is

- An overview of some of the general features of Artemis and Athena
- A highlight of a few areas where novices often go astray

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What This Talk Is Not

- An exhaustive documentation of every feature in Artemis and Athena
- A detailed tutorial
- A discussion of EXAFS theory

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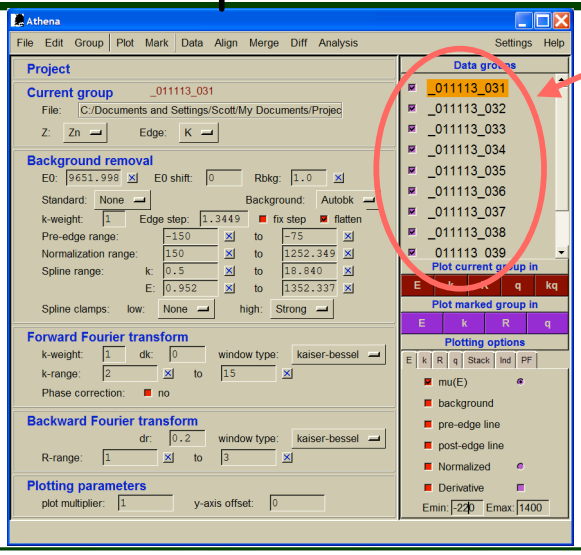
Groups in Athena



"Groups" include individual scans

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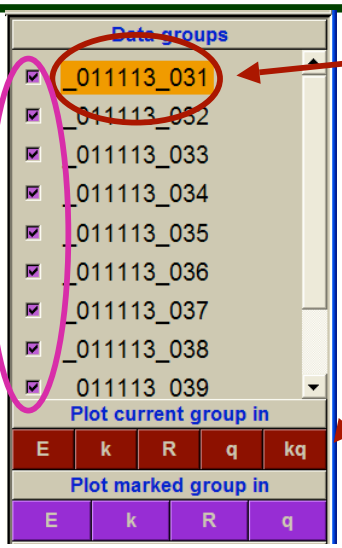
"Marked" and "Current" Groups



Checks indicate "marked" groups

This is the "current" group

Note that these buttons plot the current group

These buttons plot all the marked groups

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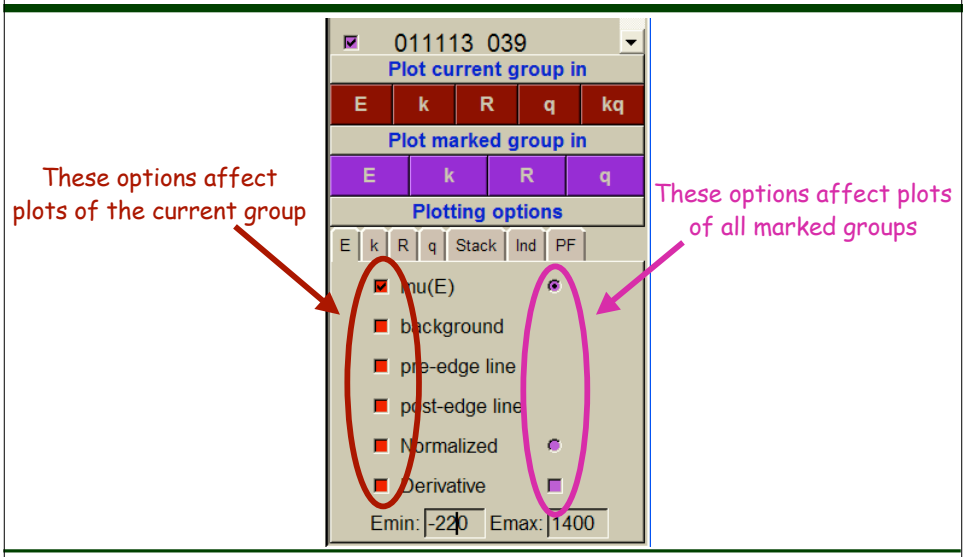
"Marked" and "Current" Groups



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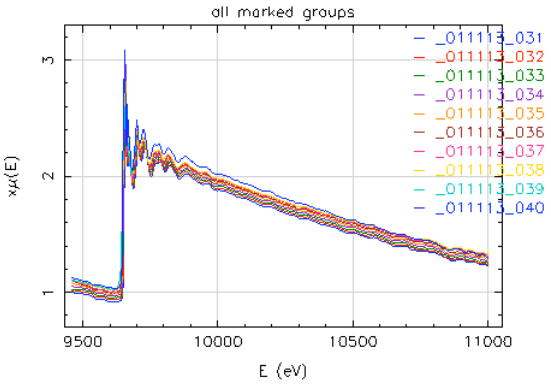
Compare Scans



Vertical translation between scans will not affect EXAFS

But a closer look…

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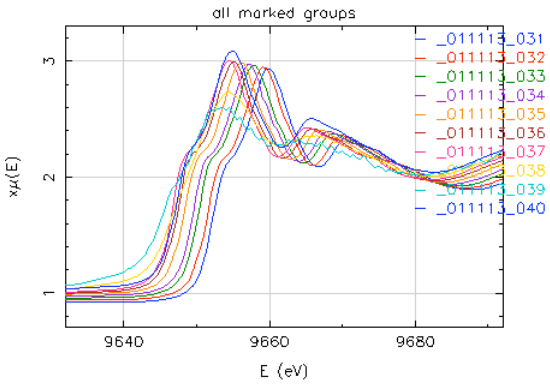
Compare Scans



...reveals other problems.

Energy calibration appears to have drifted

Scans 38 and 39 appear inconsistent with the rest

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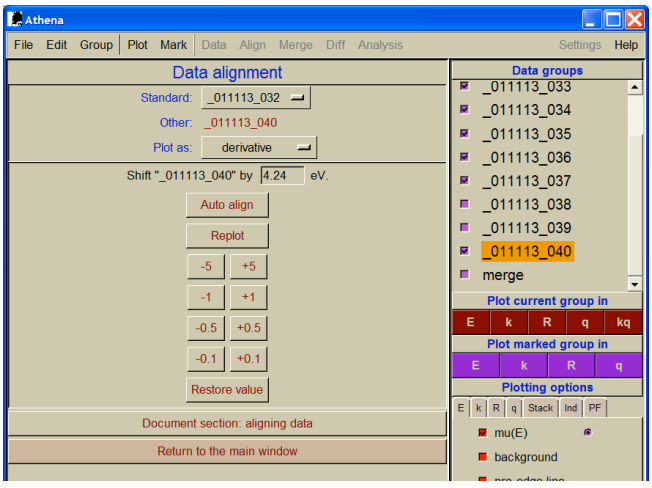
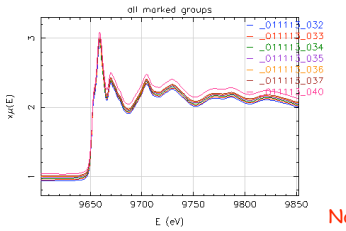
Alignment in Athena



Under the "align" menu, you can have Athena attempt to shift scans for you, or you can do it "by hand"

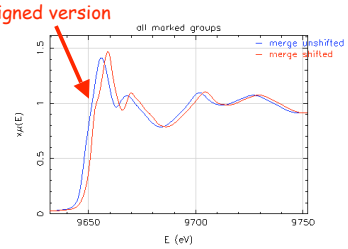
Alignment Matters



The scans are now aligned

If we had not aligned them, the average would show considerable differences:

Note missing shoulder on unaligned version



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alignment is very important

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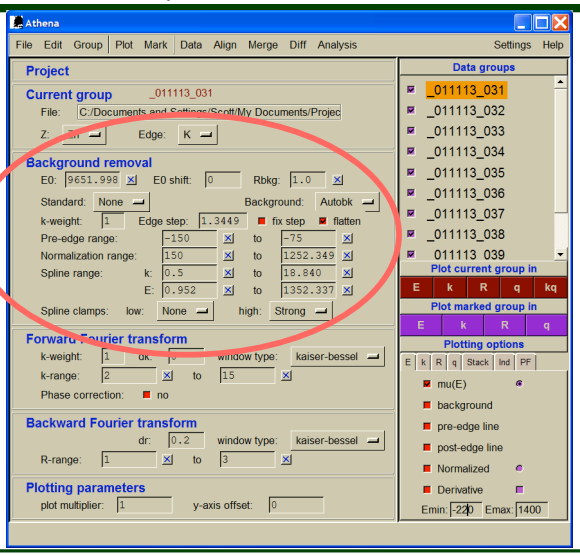
Background Removal in Athena

This information applies to the *current* scan

Right clicking brings up a menu that lets you apply these settings to all scans, or to all *marked* scans



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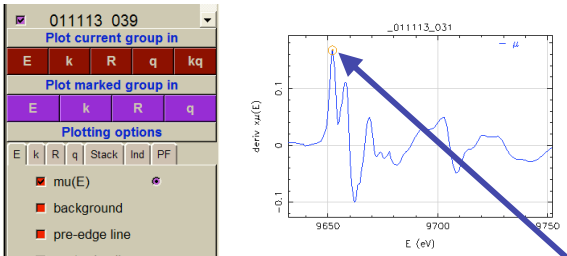
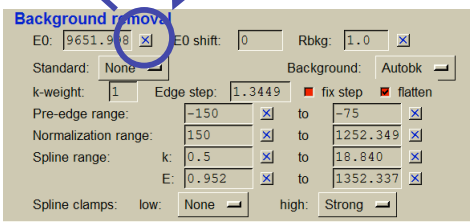
Choosing E_0 in Athena



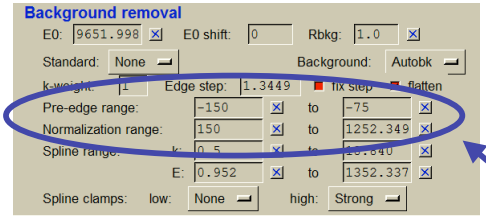
Click here to see a plot of the derivative spectrum

Choose E_0 at first peak in the derivative spectrum



Choosing E_o carefully is of low importance for EXAFS, as long as it is done consistently for all scans

Normalizing in Athena



Choose pre-edge and normalization ranges

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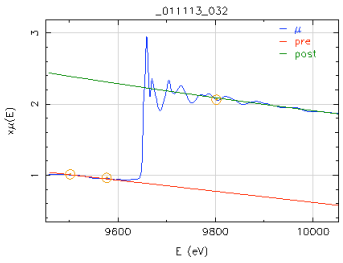
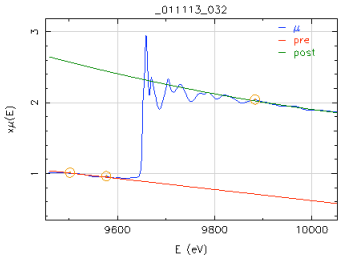
Good and Bad Normalization



These pre- and post-edge lines look OK



This post-edge line goes too high near edge

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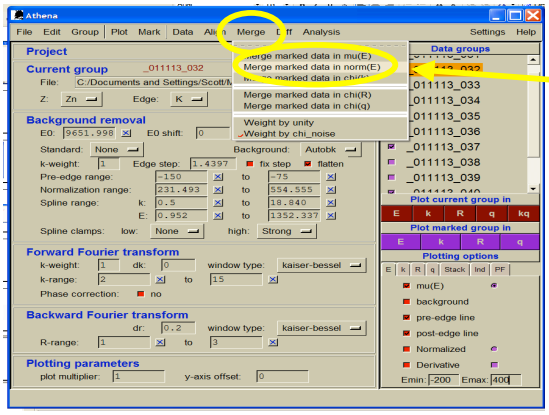
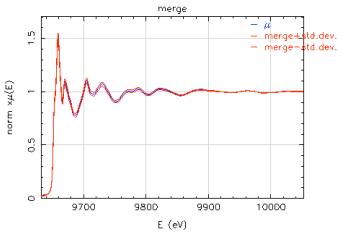
Merging Data in Athena

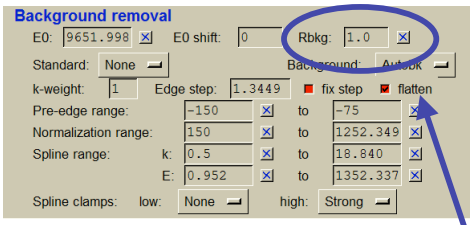


Merge aligned and normalized scans here



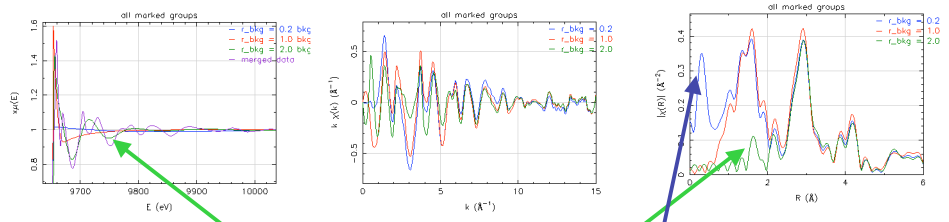
Normalization may be very important in some cases, such as determining coordination number when you think you know S_0^2, but if you are fitting S_0^2 it is relatively unimportant

R_{bkg}



R_{bkg} controls how far up in the Fourier transform the background will try to suppress; i.e. how "wiggly" the background can be

R_{bkg}



Energy plot

k-space plot

Magnitude of Fourier transform

R_{bkg} of 2.0 _ wiggles too much in energy space and thus kills off low-R peak in Fourier transform

R_{bkg} of 0.2 Å "misses" in energy space and thus introduces spurious low-R peak in Fourier transform

R_{bkg} is fairly important

Ideally, small changes in R_{bkg} should not significantly change the parameters you find via your fits

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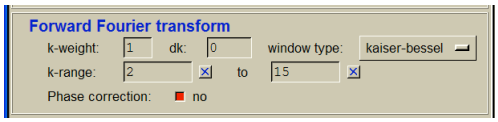
Fourier Transforms in Athena



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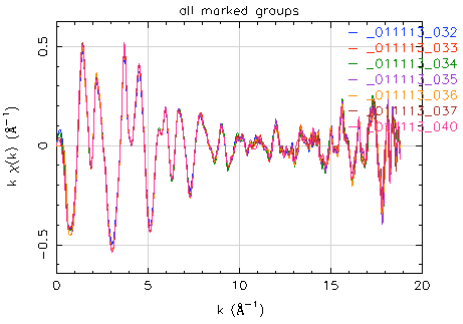
Choosing k_{max}



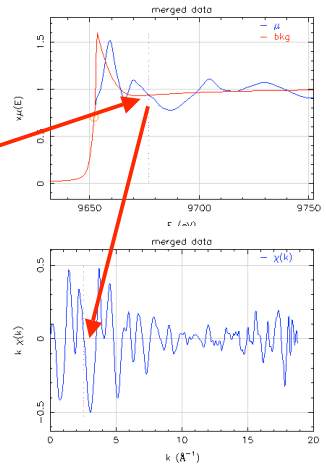
This data appears consistent for all scans. If there is trouble at high-*k*, it is systematic and reproducible.

Choice of k_{max} should be of low importance

Ideally, small changes in choice of k_{max} should not change parameters you find via your fits

Choosing k_{min}

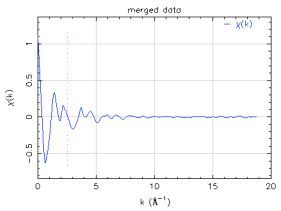
Choose k_{min} where background stops being strongly dependent on small changes in background parameters



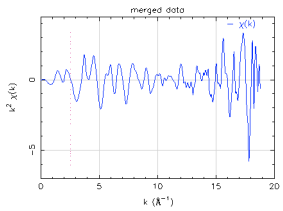
Choice of k_{min} *should* be of low importance

Ideally, small changes in choice of k_{min} should not change parameters you find via your fits. In practice, fit is often more sensitive to k_{min} than k_{max}

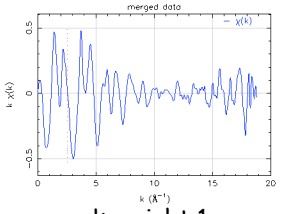
k-weight



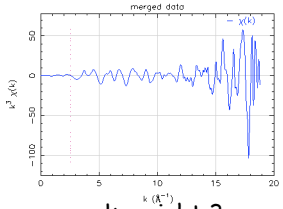
Unweighted



k-weight 2



k-weight 1



k-weight 3

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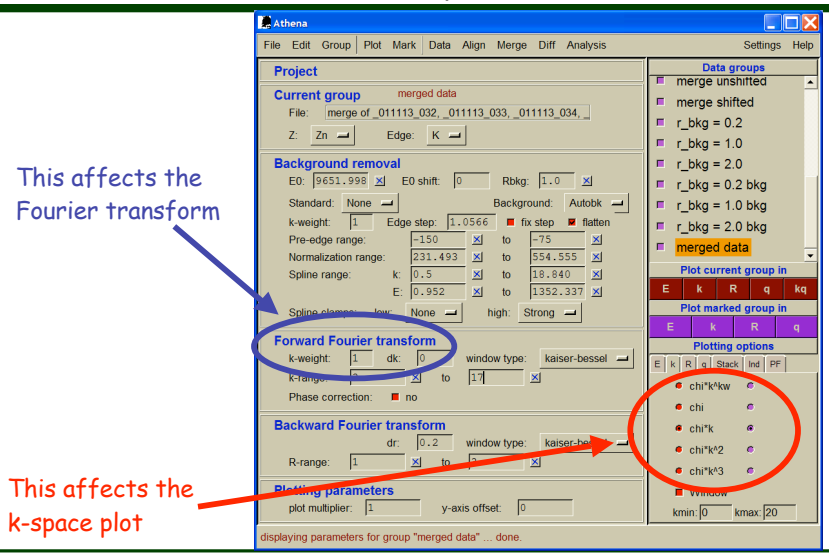
Athena Reminder!



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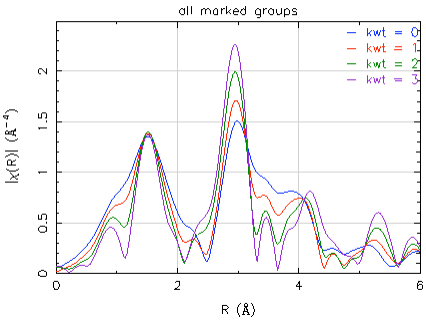
Effect of k-weight on Fourier Transform



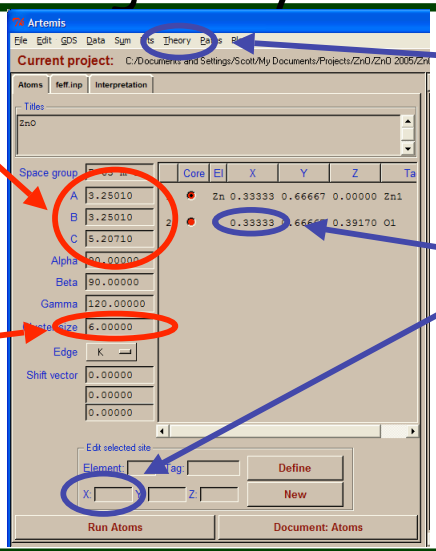
k-weight *should* be of low importance

Ideally, different k-weights should not change parameters you find via your fits.

Entering a Crystal Model

Lattice parameters are given in Angstroms

This is the maximum distance from the absorbing atom (in Angstroms) that you want feff to calculate. Make it a few Angstroms larger than the largest path you plan to use, so that feff can calculate potentials properly



Get here from the Theory menu

Artemis gives coordinates of atoms in fractional coordinates; i.e. multiply by lattice parameters to get Angstroms

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What if the Sample Isn't Crystalline?

- Short-Range Amorphous (e.g. glasses): Use a crystal structure which is locally similar on the Atoms page, but only use the inner paths for analysis
- Macromolecular: Use the space group P 1 and lattice parameters A=B=C=100. Then enter coordinates of atoms in units of hundredths of an Angstrom.

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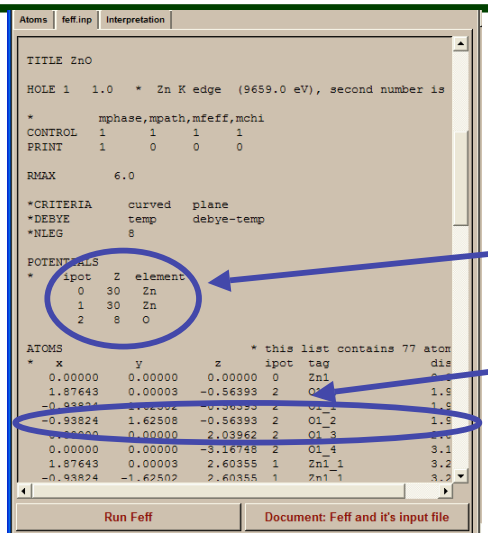
Atoms Generates a feff.inp File



This file is generated automatically when you run Atoms, but you should look at it to see if it makes sense

This list of potentials can be changed, but the absorber must be 0 and you cannot skip numbers

These coordinates and distances are given in Angstroms; you should always check that first-shell distances and coordination numbers make sense to you

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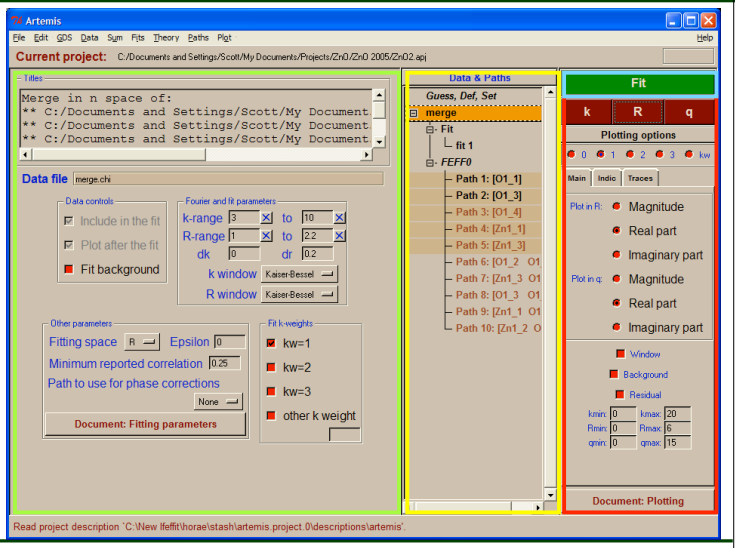
The Artemis Main Screen

The left part of the screen changes depending on what is highlighted in…
…the "Data & Paths" panel.

The right side of the screen mostly controls the plots…
…and the big green Fit button makes it go!



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Feff Screen

Interpretation shows you a list of paths:

Black non-italicised paths are included in the fit

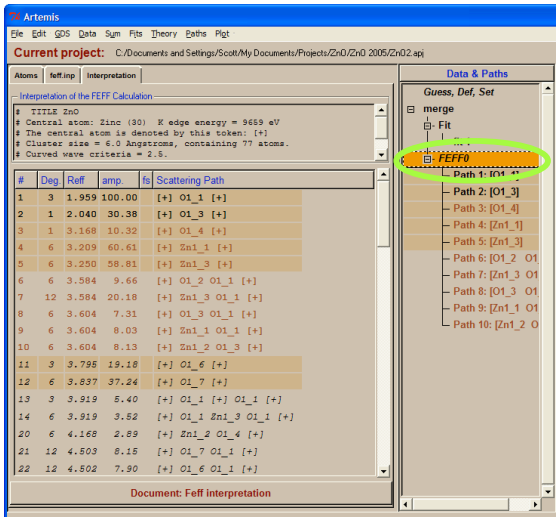
Paths with the text in brown are not currently included in the fit

Italicised black paths are not currently in the path list at all

Paths with brown backgrounds are direct scattering

Paths with blue backgrounds are focused

Right-clicking allows you to add paths to the list, include them in the fit, and more…



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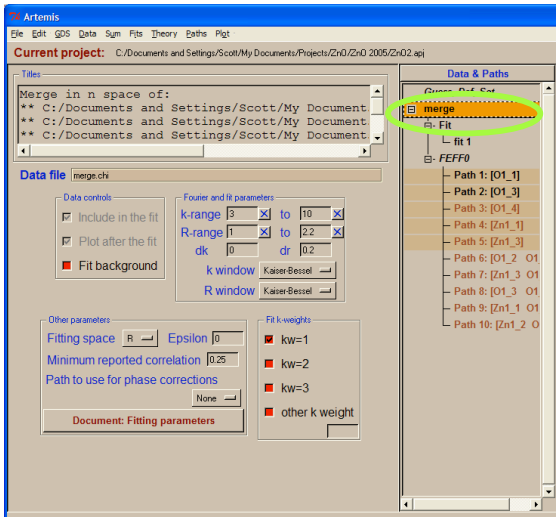
Data Screen

Clicking on a data set brings up a screen where you can choose k- and R-ranges for fit, k-weights, etc..



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Guess, Def, Set Screen

This screen allows you to define various kinds of parameters:

Guess parameters are *optimized during* fitting

Def parameters are *calculated during* fitting

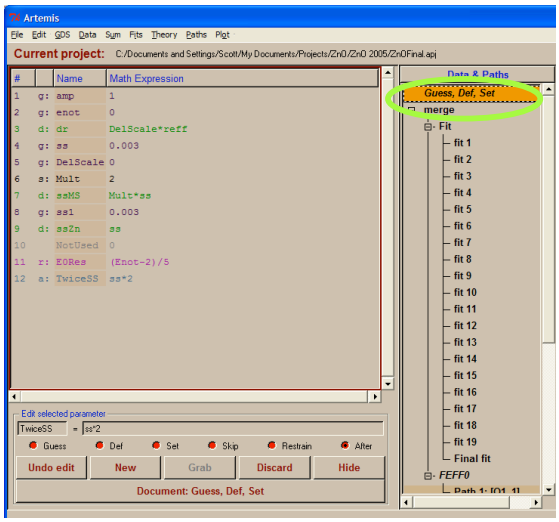
Set parameters are *calculated before* fitting

After parameters are *calculated after* fitting

Skip parameters are not used

Restraints force a parameter to be close to a specified value

"reff" is a special parameter equal to half of the nominal path length



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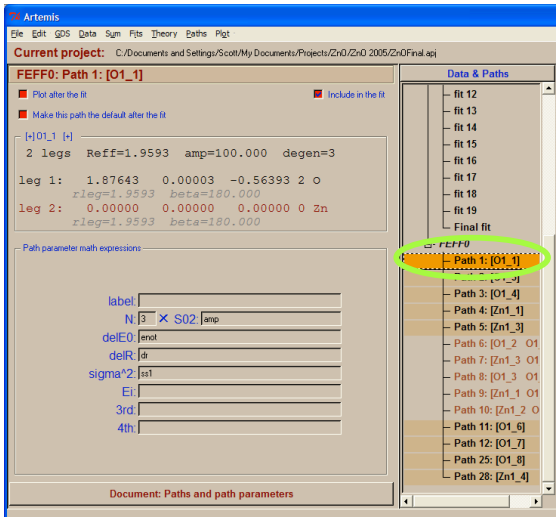
Guess, Def, Set Screen

Clicking on a path lets you specify path parameters in terms of Guess, Def, Set parameters



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Log Files Screen

Clicking on Fit in the Data & Paths screen brings up a screen that lets you view results from previous fits and compare them graphically